Itinerant Ferromagnetism in a polarized two-component Fermi gas

Pietro Massignan
ICFO - The Institute of Photonic Sciences - 08860 Castelldefels, Barcelona, Spain

Zhenhua Yu
Institute for Advanced Study, Tsinghua University, Beijing 100084, China

Georg M. Bruun
Department of Physics and Astronomy, University of Aarhus, Ny Munkegade, DK-8000 Aarhus C, Denmark

(Dated: January 16, 2013)

We analyze when a repulsively-interacting two-component Fermi gas is thermodynamically stable in a phase separated state. We focus on the strongly polarised limit where the many-body problem can be described accurately in terms of repulsive polarons and the entropy of mixing. Phase diagrams as a function of polarisation, temperature, mass imbalance, and polaron energy as well as scattering length and range parameter are provided. When extrapolated to zero polarisation, our results are consistent with Monte-Carlo calculations. The lifetime of the polaron state is shown to increase significantly with the interaction range, which raises the prospects of realizing the elusive itinerant ferromagnetic phase with ultracold atoms at a moderately narrow Feshbach resonance.

A mixture of two distinguishable species of fermions with strong repulsive interactions was predicted long ago by E. Stoner to undergo a transition towards an itinerant ferromagnetic state, where the two components phase separate to minimize the interaction energy [1]. This is a strongly interacting many-body problem, notoriously difficult to solve, as such there are many competing and often contradictory theories. Moreover, its practical implementation is far from trivial and itinerant ferromagnetism has not yet been unambiguously observed. An exciting new setting to investigate this phenomenon is provided by ultracold atomic gases, since they offer great experimental flexibility and a precise determination of physical parameters [2]. Though a recent experiment claimed the observation of itinerant ferromagnetism in a strongly repulsive Fermi gas [3], the current consensus is that fast decay precludes the realization of the ferromagnetic state for atoms interacting via a broad Feshbach resonance [4–7]. However, a major step forward in the quest to produce long-lived repulsive Fermi gases was represented by the production of a ^{6}Li-^{40}K mixture at a moderately narrow Feshbach resonance, which leads to a much smaller decay rate [8]. This raises the hope that one can in fact observe itinerant ferromagnetism in atomic gases by choosing appropriate atoms and resonances. Previous theoretical studies of itinerant ferromagnetism in the cold atom context employed mean-field, diagrammatic, and Monte-Carlo calculations [4, 6, 9–18]. The effects of a non-zero range of the interaction, which in light of their positive effect on the lifetime are highly relevant, were not examined in detail, and only in Refs. [4–6, 14] was the problem of decay considered.

In this paper, we perform a thermodynamic analysis by comparing the free energies of two possible configurations of a two-component Fermi gas, the fully mixed phase, and the partially/fully separated (ferromagnetic) phase. A key point is that we focus on the limit of strong polarisation where one can develop an accurate many-body theory in terms of repulsive polarons and the entropy of mixing. This allows us to calculate reliable phase diagrams as a function of polarisation, temperature, mass-imbalance and polaron energy as well as scattering length and range parameter. The ferromagnetic region is shown to shift toward the BCS side with increasing range parameter while the lifetime of polarons increases significantly. We finally perform a virial expansion, which confirms that the critical temperature for ferromagnetism decreases with increasing range. The substantial lifetime improvement indicates that the itinerant ferromagnetic phase might finally be realised with cold atoms interacting via moderately narrow Feshbach resonances, which are readily available experimentally.

We consider a two-component Fermi gas consisting of N_1 atoms with mass m_1 and N_2 atoms with mass m_2 in a volume V. Two atoms of different species interact repulsively ("on the upper branch") via a short-range potential in the s-wave channel, whereas the intra-species interaction can be neglected. If the system is perfectly phase separated so that the 1-atoms occupy a volume V_1 and the 2-atoms occupy a volume $V_2 = V - V_1$ with no mixing of the two species, the energy per particle is

$$\varepsilon_{\rm sep} = (1-y)\varepsilon_1(N_1/V_1, T) + y\varepsilon_2(N_2/V_2, T), \tag{1}$$

where $y = N_2/N$ is the fraction of the 2-atoms, and $N = N_1 + N_2$. The energy per particle ε_σ of an ideal Fermi gas of N_σ σ-atoms in a volume V_σ reads

$$\varepsilon_\sigma = \frac{3}{2}\frac{\mathrm{Li}_{5/2}(-z_\sigma)}{\mathrm{Li}_{3/2}(-z_\sigma)}k_BT, \tag{2}$$

where $\mathrm{Li}_x(z)$ is the polylogarithm. The fugacity $z_\sigma = \exp(\mu_\sigma/k_BT)$, with μ_σ the chemical potential, is determined by the density $n_\sigma = N_\sigma/V_\sigma$ via $n_\sigma =$

$-\text{Li}_{3/2}(z_\sigma)/\lambda_\sigma^3$ where $\lambda_\sigma = (2\pi\hbar^2/k_BTm_\sigma)^{1/2}$ is the thermal de Broglie wavelength. We recover the usual results $\varepsilon_\sigma = 3E_{F\sigma}[1+\frac{5\pi^2}{12}(k_BT/E_{F\sigma})^2]/5$ for $T \ll T_{F\sigma}$, and $\varepsilon_\sigma = 3k_BT/2$ for $T \gg T_{F\sigma}$, where $E_{F\sigma} = k_BT_{F\sigma} = \hbar^2(6\pi^2n_\sigma)^{2/3}/2m_\sigma$.

Consider next a highly polarised homogeneous mixture with $N_2 \ll N_1$. In this limit the system can be described as an ideal gas of 1-atoms, mixed with a gas of well-defined quasiparticles consisting of 2-atoms dressed by the 1-atoms. The quasiparticles are referred to as repulsive polarons and they are the many-body equivalent of the repulsive branch of a Feshbach resonance. The energy per particle in this limit is accurately given by [13]

$$\varepsilon_{\text{mix}} = (1-y)\varepsilon_1(N_1/V,T)+y\varepsilon_2(N_2/V,T)+y(1-y)^{2/3}E_+. \tag{3}$$

Here E_+ is the energy of a zero-momentum repulsive polaron in a Fermi sea of 1-atoms with density $n = N/V$ and Fermi energy $E_F = \hbar^2k_F^2/2m_1$, with $k_F = (6\pi^2n)^{1/3}$ [6]. In the low temperature regime, we may safely approximate E_+ by its value at zero temperature. The factor $(1-y)^{2/3}$ is a rescaling of the polaron energy taking into account the fact that the 2-atoms are immersed in a Fermi sea with lower density $N_1/V = (1-y)N/V$. The effective mass m_2^* of the repulsive polaron is close to m_2 [6], and we therefore take $m_2^* = m_2$ for simplicity. Fixed-node Monte-Carlo calculations indicate that the expression (3) is accurate for polarizations $P = (N_1-N_2)/(N_1+N_2) \gtrsim 0.5$, corresponding to $y \lesssim 0.25$ [13].

The thermodynamically unstable region of the homogeneous mixed phase can be determined by applying the usual Maxwell construction to the free energy per particle $f = \varepsilon - Ts$, where s is the entropy per particle. Let us first focus on the case of equal masses $m_1 = m_2 = m$. The case of $m_1 \neq m_2$ will be discussed later. For the phase separated state, equating the pressures of the two phases yields $N_1/V_1 = N_2/V_2 = n$, the total density of the system. The energy per particle (1) is then $\varepsilon_{\text{sep}} = \varepsilon(n,T)$ independent of y. Here we have dropped the subscript σ on ε_σ since $m_1 = m_2$. We can therefore perform a Maxwell construction on the difference $\Delta f = f_{\text{mix}} - f_{\text{sep}}$ which is given by

$$\Delta f = (1-y)\varepsilon(n_1)+y\varepsilon(n_2)+y(1-y)^{2/3}E_+ - \varepsilon - T\Delta s. \tag{4}$$

A major advantage of using the difference Δf is that we do not need to calculate s_{mix} for the mixed state. Instead, we can use the entropy of mixing expression $\Delta s = -k_B[y\ln y + (1-y)\ln(1-y)]$, which is the change in entropy corresponding to complete mixing of two separated ideal gases. This expression reflects the purely combinatorial effects of mixing and we therefore expect it to be accurate for $y \lesssim 0.25$, where interactions between quasiparticles are negligible (ideal mixture assumption).

In Fig. 1, we plot the phase diagram obtained from a Maxwell construction using (4) as a function of E_+ and

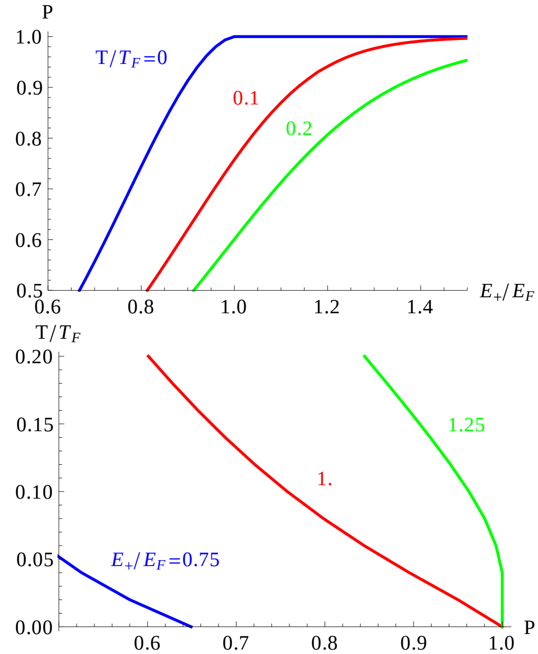

FIG. 1. Phase diagrams in terms of the polaron energy E_+, the polarization P, and the temperature T. The gas is mixed above the lines, and phase separated below.

P for various temperatures (top), and as a function of P and T for various polaron energies E_+ (bottom). We have only shown the diagram for $P \geq 1/2$ where our theory can be expected to be accurate. When $T = 0$ and $P \to 1$, Fig. 1 shows that the system phase separates when $E_+ > E_F$. This simply reflects that the 2-atoms cannot diffuse into a polaron state in the ideal gas of 1-atoms if the polaron energy is higher than the Fermi energy. For smaller polarisation P, phase separation occurs at a smaller polaron energy E_+ since the system can separate into two partially polarised phases, which reduces the kinetic energy cost. Conversely, we see that phase separation is suppressed at higher temperatures due to the entropy of mixing. Note that the phase diagram in Fig. 1 is generic in the sense that it is based only on the existence of well-defined repulsive quasi-particles with energy E_+, which has been verified experimentally [8], and on the ideal mixture assumption.

To make a direct connection with experiments, we now calculate E_+ in terms of the scattering parameters of the interaction: the s-wave scattering length a and the range parameter R^*. At the many-body level, a small/large k_FR^*, corresponds to a wide/narrow Feshbach resonance. The range parameter is $R^* = \hbar^2/(2m_ra_{\text{bg}}\delta\mu\Delta B) > 0$, where a_{bg} is the background scattering length, $\delta\mu$ is the differential magnetic moment, and ΔB the magnetic width of the Feshbach resonance. A very attractive feature of the high polarization limit is that it is possible to calculate E_+ precisely even for strong interactions [6, 8, 19–22]. The details of the many-body cal-

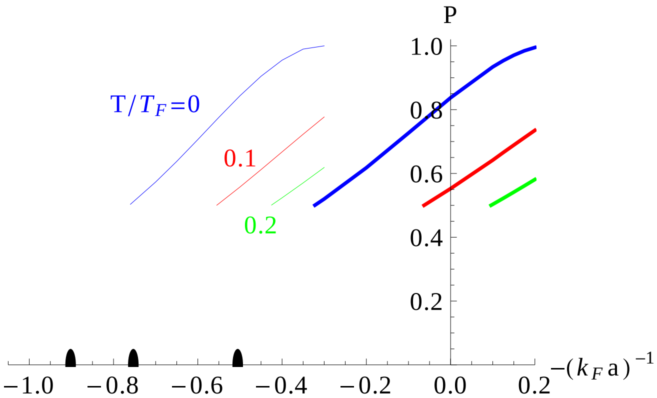

FIG. 2. Phase diagram for equal masses, at a broad resonance with $k_F R^* = 0$ (thin lines), and at a narrow one with $k_F R^* = 1$ (thick). The gas is mixed above the lines, and phase separated below. The black markers in the graph indicate the IFM transition at $P = T = R^* = 0$ as found using (from left to right) Monte-Carlo calculations [11–13], second order perturbation theory [9], and mean field (Stoner) theory [1]: $k_F a/2^{1/3} = \{0.9,\ 1.1,\ \pi/2\}$.

culation of E_+ as a function of a and R^*, which includes one particle-hole excitations from the Fermi sea of the majority atoms, can be found elsewhere [6, 8, 23].

The resulting phase diagram in terms of the scattering parameters is shown in Fig. 2. We consider two different values of the range: $k_F R^* = 0$ (thin lines) describing a wide Feshbach resonance, and $k_F R^* = 1$ (thick lines) corresponding to the intermediate value of the experiment in Ref. [8]. We observe that a non-zero effective range shifts the phase separated region toward the BCS-regime (the right side of the plot), consistent with the shift of the polaron/molecule crossing reported in Ref. [8]. As in Fig. 1, we have drawn the phase boundary lines only within the regime of validity of the polaron theory, i.e., $P > 1/2$. With increasing $-(k_F a)^{-1}$, we have furthermore terminated the lines where the polaron Ansatz fails as the polaron decay rate Γ_{PP} becomes too large, i.e., when $\Gamma_{PP}/E_F > 0.25$. The issue of the polaron decay will be discussed in more detail below. For comparison, in Fig. 2 we also give the critical values for the ferromagnetic transition for the balanced case $P = 0$ calculated by various zero-temperature theories [1, 9, 11–13]. Due to the symmetry of the phase diagram for equal masses, the phase boundary must cross the $P = 0$ axis vertically. As can be seen from Fig. 2, this significantly restricts the range of possible extrapolations of our theory from its range of validity to smaller values of $|P|$. In particular, the extrapolation of our theory to $P = 0$ is consistent with the $T = 0$ critical coupling strengths predicted by the Monte-Carlo calculations [11–13] which indicates the accuracy of our approach. Conversely, it is difficult to reconcile with mean-field Stoner theory [1].

Since a long lived repulsive polaron state has been recently achieved for a mixture of ^{6}Li and ^{40}K atoms [8], we turn now to study the effects of unequal masses $m_1 \neq m_2$. For simplicity, we consider $T = 0$ and the limit $P \to 1$ where it is sufficient to compare the energy of the mixed phase with that of the perfectly phase separated state, given respectively by (3) and (1). For the perfectly phase separated state, the pressures p_σ of the two phases must be equal; using $p_\sigma \propto (N_\sigma/V_\sigma)^{5/3}/m_\sigma$ for an ideal Fermi gas, we find $N_1/V_1 = n[y(m_1/m_2)^{3/5} + 1 - y]$ and $N_2/V_2 = n[(1-y)(m_2/m_1)^{3/5} + y]$. To first order of y, Eq. (1) becomes

$$\varepsilon_{\rm sep} = E_{F1}(n)\left[3/5 + y(m_1/m_2)^{3/5} - y\right] \qquad (5)$$

which is accurate when $y \ll 3|(m_1/m_2)^{3/5} - 1|^{-1}$. To the same order of y, Eq. (3) is of the form $\varepsilon_{\rm mix} = E_{F1}(n)\,[3/5 + y(E_+/E_{F1}(n) - 1)]$. The homogeneous mixture is unstable when $\varepsilon_{\rm mix} > \varepsilon_{\rm sep}$ which gives [6]

$$E_+ > \left(\frac{m_1}{m_2}\right)^{3/5} E_{F1}(n) = \frac{(6\pi n)^{2/3}}{2m_2^{3/5}m_1^{2/5}}. \qquad (6)$$

This result demonstrates that phase separation is favored by making one of the atom species very heavy, since the kinetic energy cost then decreases. This effect was also discussed in Refs. [15, 18].

Previous studies showed that strongly repulsive Fermi gases prepared close to a broad Feshbach resonance suffer from severe decay toward the “lower branch” [3–7]. It is therefore important to address the question: are there conditions under which a strongly repulsive Fermi gas has a sufficiently long lifetime for the observation of the ferromagnetic state? To examine this, we plot in Fig. 3(a) the critical value of the interaction parameter $1/k_F a$ for phase separation at $T = 0$ and $P \to 1$ for different mass ratios obtained from (6), and in Figure 3(b) we plot the corresponding two-body decay rate Γ_{PP} of the repulsive polaron at the critical coupling strength. The rate Γ_{PP} is calculated using a diagrammatic method including effects from a non-zero range R^*, whose results are in good agreement with experimental data [6, 8]. Figure 3 shows an important result: a narrow resonance with large $k_F R^*$ gives rise to a longer polaron lifetime than a broad one. For instance, for a mixture of a few ^{40}K atoms in a gas of ^{6}Li atoms, the mass ratio is $m_2/m_1 = 40/6$, and the polaron lifetime increases by a factor ~ 10 at the critical coupling strength for phase separation if the range of the atom-atom interaction is $k_F R^* = 1$ instead of zero. Furthermore, we find that a large mass ratio m_2/m_1 decreases the decay rate significantly compared to the case of equal masses. These results demonstrate that the decay of the repulsive phase towards the attractive branch may be strongly reduced, and as such the prospects of observing itinerant ferromagnetism increased, by employing heavy impurities in a bath of light atoms at a moderately narrow Feshbach resonance. Note that our results indicate that phase separation of an initially mixed phase is

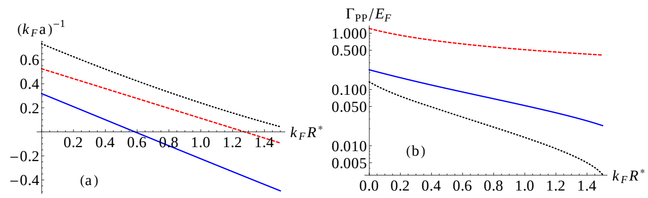

FIG. 3. (a) The critical coupling strength for phase separation for $T = 0$ and $P = 1$ as a function of R^*. (b) The decay rate $\Gamma_{\rm PP}$ of the repulsive polaron at the transition. Blue: $m_2/m_1 = 1$, black: 40/6, and red: 6/40.

unlikely due to fast decay (larger than typical trap frequencies), but that an initially separated phase should be long-lived. To investigate further the stability of the phase separated state, one could calculate the tunneling rate of atoms between the two phases taking into account not only the lifetime of the repulsive polaron but also its quasiparticle residue and the molecule-hole continuum.

We finally examine the high temperature regime, where one can obtain reliable results using the virial expansion. To second order, this expansion gives for the partition function of the two-component Fermi gas

$$\mathcal{Z} = 1 + V\sum_{\sigma=1,2}\frac{z_\sigma}{\lambda_\sigma^3} + \frac{V}{2}\left(\sum_{\sigma=1,2}\frac{z_\sigma}{\lambda_\sigma^3}\right)^2 + \frac{V z_1 z_2 b_2}{\lambda_M^3}, \quad (7)$$

with $M = m_1 + m_2$, $1/m_r = 1/m_1 + 1/m_2$, $\lambda_r = (2\pi\hbar^2/2k_BTm_r)^{1/2}$, and $\lambda_M = (2\pi\hbar^2/k_BTM)^{1/2}$. When only the s-wave "upper branch" of excitations is taken into account, the second virial coefficient b_2 is [24]

$$b_2 = \frac{1}{m_rT}\int_0^\infty \frac{dk}{\pi} k\delta_s(k)e^{-k^2/2m_rT}. \quad (8)$$

The s-wave phase shift is given by $\cot\delta_s(k) = -1/ka - R^*k$. At a broad resonance one has $b_2 = e^{(\lambda_r/2\sqrt{\pi}a)^2}\left[1 + \mathrm{erf}(\lambda_r/2\sqrt{\pi}a) - 2\theta(a)\right]/2$, whose minimum value is $-1/2$ at $1/a = 0^+$. For a very narrow resonance, we find $b_2 \sim -\lambda_r/2\pi R^*$ at the unitary point.

The free energy per particle of the mixture $f_{\rm mix} = -k_BT\ln\mathcal{Z}/N + (1-y)\mu_1 + y\mu_2$ is

$$\begin{aligned} f_{\rm mix} = -k_BT\{&1 - (1-y)\ln[(1-y)n\lambda_1^3] - y\ln(yn\lambda_2^3) \\ &+ y(1-y)n\lambda_r^3 b_2\}, \end{aligned} \quad (9)$$

where we have used $z_\sigma = \lambda_\sigma^3(n_\sigma - \lambda_r^3 n_1n_2b_2)$ obtained from (7). The phase diagram will have a phase separated region when

$$\partial_y^2 f_{\rm mix}/k_BT = (1-y)^{-1} + y^{-1} + 2n\lambda_r^3 b_2 \le 0, \quad (10)$$

for some values of y, which is possible only if $b_2 < 0$. For equal masses, the region of phase separation derived from the Maxwell construction is bounded by the concentrations which minimise $f_{\rm mix}$, i.e.,

$$\partial_y f_{\rm mix}/k_BT = \ln[y/(1-y)] + (2y-1)n\lambda_r^3 b_2 = 0. \quad (11)$$

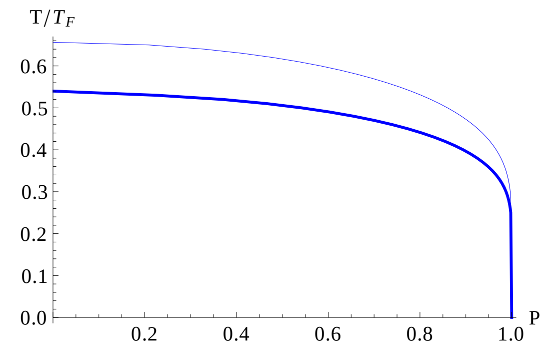

FIG. 4. Phase diagram at the unitarity point $a^{-1} = 0$ for equal masses as obtained from the virial expansion to second order: $k_FR^* = 0$ (thin line) and $k_FR^* = 1$ (thick). The gas is mixed above the lines, and phase separated below.

The phase diagram obtained from (11) is plotted in Fig. 4 for $(k_Fa)^{-1} = 0$, $m_1 = m_2$, and $k_FR^* = 0$ or $k_FR^* = 1$. Since there is no kinetic energy cost of phase separation for high temperatures, this phase diagram is a result of the competition between the repulsive interaction energy and the entropy of mixing. The predicted critical temperature for phase separation unfortunately is too low for the virial expansion to be reliable. Indeed, the largest transition temperature is $T_c^{\rm max} \approx 0.66T_F$ obtained at unitarity for a broad resonance where $b_2 = -1/2$. The calculation nevertheless indicates that a large range decreases the critical temperature for phase separation, consistently with the low temperature polaron calculation.

To conclude, we derived detailed phase diagrams of a two component Fermi gas in the limit of strong polarisation, where the effects of the interactions can be accurately described in terms of the repulsive polaron energy and the entropy of mixing. This phase diagram was then expressed in terms of the scattering length and range parameter using a many-body theory known to be reliable in the strongly polarised limit. The ferromagnetic region was shown to move towards the BCS side with increasing range of the interaction. Importantly, a large range furthermore increases substantially the polaron lifetime, raising hopes for the realisation of itinerant ferromagnetism in a physical system.

Insightful discussions with M. Zaccanti, T.-L. Ho and M. Lewenstein are gratefully acknowledged. This research has been funded through ERC Advanced Grant QUAGATUA, Spanish MEC project TOQATA, Tsinghua University Initiative Scientific Research Program, NSFC under Grants 11104157 and 11204152, the Carlsberg Foundation and the ESF POLATOM network.

[1] E. Stoner, Philos. Mag. **15**, 1018 (1933).

[2] S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **80**, 1215 (2008).
[3] G.-B. Jo *et al.*, Science **325**, 1521 (2009).
[4] D. Pekker *et al.*, Phys. Rev. Lett. **106**, 050402 (2011).
[5] S. Zhang and T.-L. Ho, New Journal of Physics **13**, 055003 (2011).
[6] P. Massignan and G. M. Bruun, EPJD **65**, 83 (2011).
[7] C. Sanner *et al.*, Phys. Rev. Lett. **108**, 240404 (2012).
[8] C. Kohstall *et al.*, Nature **485**, 615 (2012).
[9] R. A. Duine and A. H. MacDonald, Phys. Rev. Lett. **95**, 230403 (2005).
[10] L. J. LeBlanc, J. H. Thywissen, A. A. Burkov, and A. Paramekanti, Phys. Rev. A **80**, 013607 (2009).
[11] G. J. Conduit, A. G. Green, and B. D. Simons, Phys. Rev. Lett. **103**, 207201 (2009).
[12] S.-Y. Chang, M. Randeria, and N. Trivedi, Proc. Nat. Acad. Sci. **108**, 51 (2011).
[13] S. Pilati, G. Bertaina, S. Giorgini, and M. Troyer, Phys. Rev. Lett. **105**, 030405 (2010).
[14] D. Pekker and E. Demler, Lecture Notes of the Les Houches Summer School, Volume 94 (2012).
[15] C. W. von Keyserlingk and G. J. Conduit, Phys. Rev. A **83**, 053625 (2011).
[16] L. He and X.-G. Huang, Phys. Rev. A **85**, 043624 (2012).
[17] F. Palestini, P. Pieri, and G. C. Strinati, Phys. Rev. Lett. **108**, 080401 (2012).
[18] X. Cui and T.-L. Ho, arXiv:1208.2211 (2012).
[19] R. Combescot, A. Recati, C. Lobo, and F. Chevy, Phys. Rev. Lett. **98**, 180402 (2007).
[20] N. Prokof'ev and B. Svistunov, Phys. Rev. B **77**, 020408 (2008).
[21] R. Combescot and S. Giraud, Phys. Rev. Lett. **101**, 050404 (2008).
[22] F. Chevy and C. Mora, Reports on Progress in Physics **73**, 112401 (2010).
[23] P. Massignan, Europhys. Lett. **98**, 10012 (2012).
[24] K. Huang, *Statistical Mechanics*, 2 ed. (John Wiley & Sons, New York, 1987).